

Machine Learning
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1 Introduction

1.1 What is Machine Learning

1. Machine Learning

- Grew out of work in Artificial Intelligence (AI)
- New capabilities for computers

2. Examples:

- database mining
- applications can't program by hand (handwriting recognition, Natural Language Processing (NLP), Computer Vision)
- Neuromorphic applications

3. Definition

- Arthur Samuel(1959)

Machine Learning: Field of study that gives computers the ability to learn without being explicitly programmed.

- Tom Mitchell(1998)

Well-posed Learning Problem: A computer program is said to learn from experience E with respect to some task T and some performance measure P , if its performance on T , as measured by P , improves with experience E .

4. Machine Learning in this course:

- (a) Supervised Learning
- (b) Unsupervised Learning
- (c) Others: reinforcement learning, recommender systems
- (d) Practical application techniques

1.2 Supervised Learning

In supervised learning, the *the right answer* is given. For example:

1. Regression: predict real-valued output.
2. Classification: predict discrete-valued output.

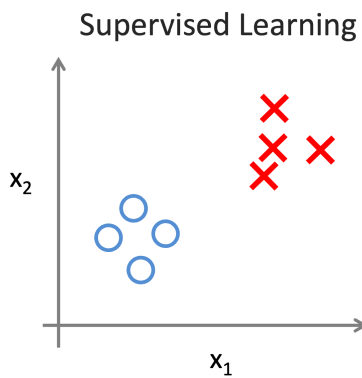


Figure 1: Supervised Learning

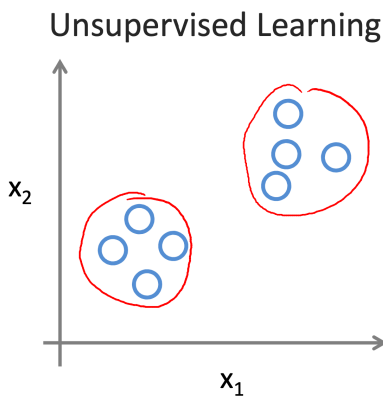


Figure 2: Unsupervised learning

1.3 Unsupervised Learning

The right answer is not given, e.g. cocktail problem (distinguishing two voices from an audio file.)

2 Linear Regression with One Variable

2.1 Model Representation

2.1.1 Notations

For a training set:

- \mathbf{m} = Number of training examples.
- \mathbf{x} = “input” variable / features.

- y = “output” variables / “target” variable.
- (x,y) - one training example.
- (x^i,y^i) denotes the i^{th} training example

2.1.2 Hypothesis Function

A hypothesis function (h) maps input (x) to estimated output (y). How do we represent h ?

Hypothesis Function $h_{\theta}(x) = \theta_0 + \theta_1 x$	(1)
--	-----

We can apply *Univariate linear regression* with respect to x .

2.2 Cost Function

Recall 1. The θ_i s are parameters we have to choose. The intuition is is that we want to choose θ_i s such that h_{θ} is closest to y for our training examples (x,y) .

Cost Function $J(\theta_0, \theta_1) = \frac{1}{2m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)})^2$	(2)
--	-----

Summary

1. **Hypothesis** $h_{\theta}(x) = \theta_0 + \theta_1 x$
2. **Parameters** θ_0, θ_1
3. **Cost Function** $J(\theta_0, \theta_1) = \frac{1}{2m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)})^2$
4. **Goal** $\min_{\theta_0, \theta_1} J(\theta_0, \theta_1)$

2.3 Gradient Descent

2.3.1 Intuition

1. We have some function $J(\theta_0, \theta_1)$, we want to $\min_{\theta_0, \theta_1} J(\theta_0, \theta_1)$
2. Outline: start with some θ_0, θ_1 , keep changing θ_0, θ_1 to reduce $J(\theta_0, \theta_1)$ until we end up at a minimum.

2.3.2 Gradient Descent Algorithm

Algorithm

repeat until convergence{

$$\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta_0, \theta_1) \quad (\text{for } j=0 \text{ and } j=1).$$

}

Notes

1. the $:=$ denotes non-blocking assignment, i.e. simultaneously updates θ_0 and θ_1
2. We use the derivative to find a local minimum.
3. α denotes the learning rate. Gradient descent can converge to a local minimum even when the learning rate α is fixed. As we approach a local minimum, gradient descent will automatically take smaller steps. Therefore it is not needed to decrease α over time.

2.3.3 Gradient Descent with Linear Regression

Recall, we have:

1. Gradient Descent Algorithm:

repeat until convergence{

$$\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta_0, \theta_1) \quad (\text{for } j=0 \text{ and } j=1).$$

}

2. Linear Regression Model:

$$h_{\theta}(x) = \theta_0 + \theta_1 x$$

$$J(\theta_0, \theta_1) = \frac{1}{2m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)})^2$$

We can substitute the above equations, which gives us:

$$\theta_0 := \theta_0 - \alpha \frac{1}{m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)})$$

$$\theta_1 := \theta_1 - \alpha \frac{1}{m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)}) \cdot x^{(i)}$$

3 Review of Linear Algebra

This section is a basic review of linear algebra. I have skipped this section for now and will come back to it if time permits.

4 Linear Regression with Multiple Variables

4.1 Multiple features

Recall in the single variable case, we have a single input (x), two parameters(θ_0, θ_1). The hypothesis can be expressed as:

$$h_{\theta}(x) = \theta_0 + \theta_1 x.$$

Now, consider a generalized case where there are multiple features: X_1, X_2, X_3 . The information can be organized in a table with example numerical values:

Sample Number (i)	X_1	X_2	y
1	6	87837	787
2	7	78	5415
3	545	778	7507
4	545	18744	7560
5	88	788	6344

Table 1: Sample Table

From Table 1, one can see that each row is a sample a feature on each column.

4.1.1 Notation

1. n : number of features.
2. $\mathbf{x}^{(i)}$: (row vector) input features of the i^{th} training example. $i = 1, 2, \dots, m$.
3. $\mathbf{x}^{(i)}_j$: value of feature j in the i^{th} training example. $j = 1, 2, \dots, n$.

4.1.2 Hypothesis

Previously,

$$h_{\theta}(x) = \theta_0 + \theta_1 \cdot x$$

Now, we can extend the hypothesis to :

$$h_{\theta}(x) = \theta_0 \cdot 1 + \theta_1 \cdot x_1 + \theta_2 \cdot x_2$$

For convenience of notation, let's define $x_0=1$, i.e. $x_0^i=1 \forall i$.

Therefore, we have: $\mathbf{x} = \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$ and $\theta = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \vdots \\ \theta_n \end{bmatrix}$. Then, the hypothesis function can be written as:

$$\begin{aligned} h_{\theta}(x) &= \begin{bmatrix} \theta_0 & \theta_1 & \theta_2 & \dots & \theta_n \end{bmatrix} \cdot \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} \\ &= \theta^T \cdot \mathbf{x} \end{aligned} \tag{3}$$

This is *Multivariate linear regression*.

4.2 Gradient Descent for Multiple Variables

4.2.1 Algorithm

Summary for Multivariables

1. **Hypothesis** $h_{\theta}(x) = \theta^T \cdot \mathbf{x}$
2. **Parameters** θ
3. **Cost Function** $J(\theta) = \frac{1}{2m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)})^2$
4. **Goal** $\min_{\theta} J(\theta)$

Gradient Descent for Multiple Variables

repeat until convergence {

$$\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta) \quad (\text{for } j=0, 1, \dots, n)$$

}

$$\theta_j := \theta_j - \alpha \frac{1}{m} \sum_{i=1}^m (h_{\theta}(\mathbf{x}^{(i)}) - y^{(i)}) \cdot x_j^{(i)}$$

Note: $x_0^{(i)} = 1$, by definition.

4.2.2 Vectorized Implementation

One can work out the linear algebra and arrive at the following simplification using vectorized operations. The cost function J can be expressed as:

$$J(\theta) = \frac{1}{2m}(\mathbf{X}\theta - \mathbf{y})^T(\mathbf{X}\theta - \mathbf{y}) \quad (4)$$

The MATLAB implementation is as follows:

```
m = length(y); % calculate how many samples
J = 1/(2*m)*((X*theta-y)')*(X*theta-y);
```

Gradient descent can be vectorized in the form:

$$\theta = \theta - \frac{\alpha}{m} \cdot \mathbf{X}^T \cdot (\mathbf{X}\theta - \mathbf{y}) \quad (5)$$

The MATLAB implementation is as follows:

```
m = length(y); % number of training examples
for iter = 1:num_iters
    theta = theta - alpha/m * X.'*(X*theta-y);
```

4.3 Gradient Descent in Practise I: Feature Scaling

- Idea: ensure each feature are on a similar scale
- Get every feature into approx. $-1 \leq x_i \leq 1$ (\sim order)
- **Mean Normalization:** Replace x_i with $\frac{x_i - \mu_i}{s_i}$, where μ_i and s_i are the sample mean and standard deviation, respectively.

4.4 Gradient Descent in Practise II: Learning Rate

- Ensure gradient descent is working: plot J_θ over each number of iteration (not over θ !)
- Example automatic convergence test: for sufficiently small α J_θ should decrease by less than 10^{-3} i one iteration.
- If α is too small, gradient descent can be slow to converge.
- If α is too large, gradient descent may not converge.
- To choose α , try 0.001, 0.003, 0.01, 0.03, 0.1, 0.3, 1... (by 3x)

4.5 Features and Polynomial Regression

We can fit into different polynomials by choice, using multivariate regression. Recall

$$h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_3$$

Let x_1 be x^1 , x_2 be x^2 , x_3 be x^3 . Note we should still apply feature scaling to x_1 , x_2 , and x_3 individually!

4.6 Normal Equation

The normal equation provides a method to solve for θ analytically. For our data with m samples, n features, recall each sample can be written as:

$$\mathbf{x}^{(i)} = \begin{bmatrix} x_0^{(i)} \\ x_1^{(i)} \\ x_2^{(i)} \\ \vdots \\ x_j^{(i)} \\ \vdots \\ x_n^{(i)} \end{bmatrix}$$

We can construct a design matrix:

$$\mathbf{X} = \begin{bmatrix} \text{---} & (x^{(1)})^T & \text{---} \\ \text{---} & (x^{(2)})^T & \text{---} \\ \text{---} & (x^{(3)})^T & \text{---} \\ & \vdots & \\ \text{---} & (x_m^T) & \text{---} \end{bmatrix} \quad (6)$$

Then θ can be found by the normal equation:

$$\theta = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y} \quad (7)$$

Normal equation is useful as no α is required to and we do not need to iterate. However, we do have to compute $(X^T X)^{-1}$, which can be computationally expensive when n is large. The complexity is $O(n^3)$ for inverse operations. Gradient Descent is useful when n is large (many features).

4.7 Normal Equation and Non-invertibility

What if $(X^T X)^{-1}$ is non-invertible?

- Redundant features (linearly dependent), i.e. having same information in two different units.
- Too many features (i.e. $m \leq n$). Delete some features or use regularization

5 Octave/MATLAB Tutorial

6 Logistic Regression

6.1 Classification

- Binary Classification: $y \in \{0, 1\}$, where 0 denotes the negative class; 1 denotes the positive class.

- Multi-class Classification: $y \in \{0, 1, \dots, n\}$

We will be using binary classification:

- Linear regression is not suitable for classification: since $h_\theta(x)$ can output out of range, i.e. < 0 or > 1 .
- We will use **logistic regression**, which ensures that the output $h_\theta(x)$ is between 0 and 1.

6.2 Hypothesis Representation

6.2.1 Logistic function

The idea is to have $0 \leq h_\theta(x) \leq 1$. Instead of the linear regression hypothesis: $h_\theta(x) = \theta^T x$, we will let:

$$h_\theta(x) = g(\theta^T x),$$

where

$$g(z) = \frac{1}{1 + e^{-z}}$$

$g(z)$ is known as the **logistic function**, also known as the Sigmoid function.

Figure 3 shows a plot of the logistic function, which ranges from 0 to 1.

which yields

$$h_\theta(x) = \frac{1}{1 + e^{-z}} \quad (8)$$

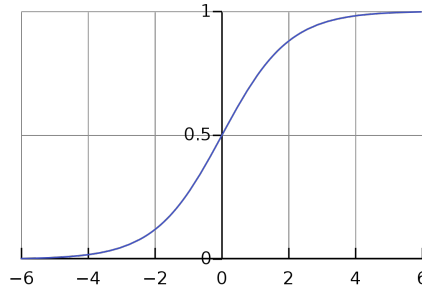


Figure 3: Sigmoid Function

6.2.2 Interpretation of Hypothesis Output

$h_\theta(x)$ = estimated probability that $y = 1$ on input x . For example, $h_\theta(x) = 0.7$ gives us a probability of 70% that the output is 1. From a probability theory point of view, one can express $h_\theta(x)$ as $P(y = 1 | x; \theta)$.

Note that since this is a probability and the total probability sums up to 1, and the real y can only be either 0 or 1:

$$P(y = 0 | x; \theta) + P(y = 1 | x; \theta) = 1$$

6.3 Decision Boundary

Recall so far we have $h_\theta(x) = g(\theta^T x)$ and $g(z) = \frac{1}{1+\exp(-z)}$. Suppose we set $h_\theta(x) = 0.5$ to be our determining factor for whether $y=0$ or $y=1$. Note that from 3, one can observe that $h_\theta(x) = 0.5$ corresponds to $\theta^T x = 0$, which is the **decision boundary**. The decision boundary is the equation which separates the different classes on a plot. There are linear and non-linear decision boundaries.

6.4 Cost function

Previously, we had $J(\theta) = \frac{1}{m} \sum_{i=1}^m \text{Cost}(h_\theta(x^{(i)}), y^{(i)})$, where $\text{Cost}(h_\theta(x), y) = \frac{1}{2}(h_\theta(x) - y)^2$. Now, the definition of the hypothesis h_θ has changed to $\frac{1}{1+\exp(-\theta^T x)}$, as a result the cost function is now non-convex.

Logistic Regression Cost Function

Therefore, a new cost function definition is needed. We propose:

$$\text{Cost}(h_\theta(x), y) = \begin{cases} -\log(h_\theta(x)) & \text{if } y = 1 \\ -\log(1 - h_\theta(x)) & \text{if } y = 0 \end{cases}$$

Note that $\text{Cost}=0$, if $y=1$, $h_\theta(x) = 1$; but as $h_\theta(x) \rightarrow 0$, then $\text{Cost} \rightarrow \infty$. This proposition captures the intuition that if $h_\theta(x) = 0$, predict $P(y = 1 | x; \theta)$, but y ends up being 1, we will penalize the learning algorithm by very large cost.

6.5 Simplified Cost Function and Gradient Descent

Since y can only be either 0 or 1, we can simplify the cost function.

$$\begin{aligned} J(\theta) &= \frac{1}{m} \sum_{i=1}^m \text{Cost}(h_\theta(x^{(i)}), y^{(i)}) \\ &= \frac{-1}{m} \left[\sum_{i=1}^m y^{(i)} \log h_\theta(x^{(i)}) + (1 - y^{(i)}) \log (1 - h_\theta(x^{(i)})) \right] \end{aligned} \tag{9}$$

Equation 9 is based on Maximum Likelihood Estimation.

A vectorized implementation is, for a design matrix \mathbf{X} :

$$\boxed{h = g(\mathbf{X}\theta)} \tag{10}$$

$$\boxed{J(\theta) = \frac{1}{m} (-y^T \log(h) - (1 - y)^T \log(1 - h))} \tag{11}$$

For gradient descent, we would want to $\min_\theta J(\theta)$:

Repeat {

$$\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta)$$

}

We can compute the partial derivative of $J(\theta)$, which is identical to that of linear regression:

$$\frac{\partial}{\partial \theta_j} J(\theta) = \frac{1}{m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)}) \cdot x^{(i)}$$

However, in this case the hypothesis function $h_{\theta}(x) = \frac{1}{1+\exp(-\theta^T x)}$ has changed!

A vectorized implementation for this is:

$$\theta := \theta - \frac{\alpha}{m} \mathbf{X}^T (g(\mathbf{X}\theta) - \mathbf{y}) \quad (12)$$

6.6 Advanced Optimization

6.6.1 Taking a Step Back

If we take a step back, and consider essentially what tasks we are performing. We need to compute two things:

1. $J(\theta)$
2. $\frac{\partial}{\partial \theta_j} J(\theta)$

6.6.2 Optimization Algorithm

There exists other more sophisticated and faster ways to optimize θ instead of gradient descent; they often do not involve selecting learning rate α and are more efficient. However, these algorithms are harder to code by hand. It is suggested that we use libraries for such algorithms.

We can write a single function that returns both $J(\theta)$ (jVal) and $\frac{\partial}{\partial \theta_j} J(\theta)$ (gradient):

```
function [jVal, gradient] = costFunction(theta)
    jVal = [...code to compute J(theta)...];
    gradient = [...code to compute derivative of J(theta)...];
end
```

Then we can use octave's "fminunc()" optimization algorithm along with the "optimset()" function that creates an object containing the options we want to send to "fminunc()".

```
options = optimset('GradObj', 'on', 'MaxIter', 100);
initialTheta = zeros(2,1);
[optTheta, functionVal, exitFlag] = fminunc(@costFunction,
    initialTheta, options);
```

We then give to the function "fminunc()" our cost function, our initial vector of theta values, and the "options" object that we created beforehand.

6.7 Multiclass Classification: One-vs-All

Now, let's extend the binary classification of data to multi-classes, i.e expanding our definition of y s.t. $y=\{0, 1, \dots, n\}$. We will divide our problem into $n+1$ ($0 \dots n$) binary classification problems. In each problem, we predict the probability that y is a member of one of our class. We train a logistic regression classifier $h_{\theta}^{(i)}(x) \forall i$ to predict $y = i$:

$$h_{\theta}^{(i)}(x) = P(y = i | x; \theta) \quad (13)$$

Figure 4 shows an example of the procedure of classifying three classes. We choose one class and then lump all the others into a single second class (hence the name One-vs-All). We apply the binary logistic regression repeatedly and use the hypothesis that returns the highest value.

$$prediction = \max_i (h_{\theta}^{(i)}(x)) \quad (14)$$

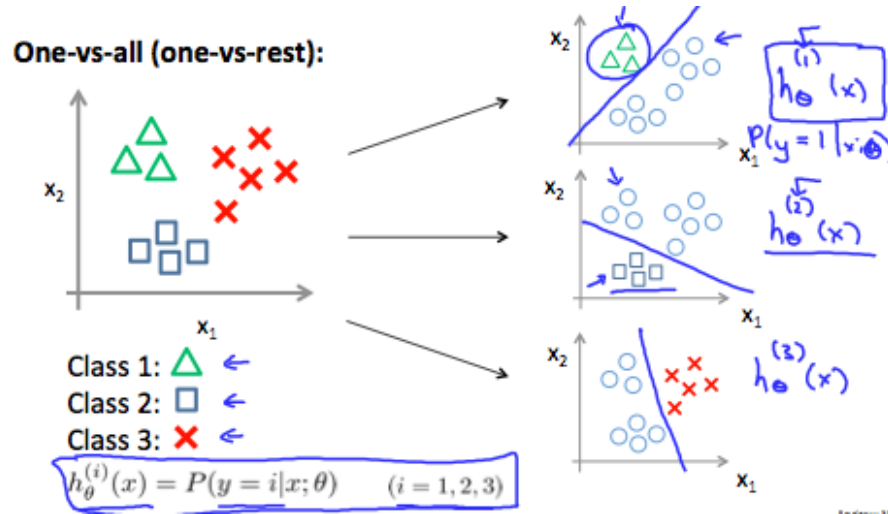


Figure 4: Example of Multiclass Logistic Regression

7 Regularization

7.1 The problem of overfitting

There are two types of errors in fitting functions to data, in which data shows the structure is not captured by the model. The terminology applies to both linear and logistic regression. Figure 5 shows an example of each fitting case.

1. Underfitting (high bias): when the form of our hypothesis function ($h_{\theta}(x)$) maps poorly to the trend of data. It is usually caused by a function that is either too simple or uses too little features.
2. Overfitting (high variance): when hypothesis function learns the training set very well hence fits the available data but does not generalize well to predict new data, i.e fitting too many details. It is usually caused by a complicated function that creates a lot of unnecessary curves and angles unrelated to the data.

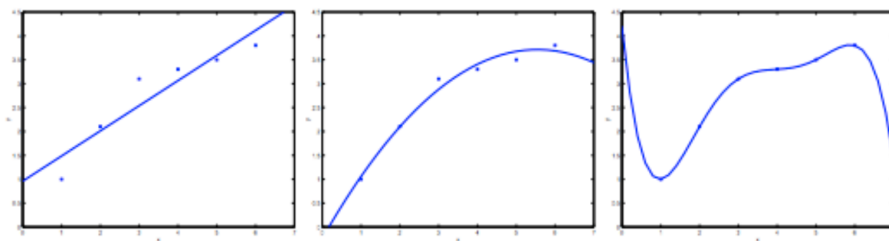


Figure 5: Three scenarios of fitting: underfit(left), good fit (middle), and overfit(right).

There are two main options to address the issue of overfitting:

1. Reduce the number of features
 - manually select which features to keep.
 - Use a model selection algorithm (later in the course).
2. **Regularization**
 - Keep all the features, but reduce the magnitude of parameters θ_j
 - Regularization works well when we have a lot of slightly useful features. (Each contributes a bit to predict y)

7.2 Cost Function

7.2.1 Intuition

Suppose we have overfitting, we can reduce the weight that some of the terms in our function carry by penalizing the feature parameter with increased cost. Consider the following hypothesis function :

$$\theta_0 + \theta_1 x + \theta_2 x^2 + \theta x^3 + \theta x^4.$$

We would want to make the function more quadratic, which means we would like to reduce the influence of θ_3 and θ_4 . Since our goal was to minimize the cost function $J(\theta)$, we could modify the original cost function

$$\min_{\theta} \frac{1}{2m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)})^2 + 1000 \cdot \theta_3^2 + 1000 \cdot \theta_4^2.$$

This will force θ_3 and θ_4 to be close to zero, and make the original hypothesis function more quadratic.

7.2.2 Regularization

Now, we can take a step further and regularize all theta parameters:

$$\min_{\theta} \left[\frac{1}{2m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)})^2 \right] + \lambda \sum_{j=1}^n \theta_j^2 \quad (15)$$

Here we are performing two separate operations which can be observed as the two terms in Equation 15. The first term corresponds to “training the data”, and the second term relates to “keeping the parameters small”. The coefficient λ is the **regularization parameter** and determines the balance between the aforementioned two objectives. Note that if λ is too big ($\approx 10^{10}$), then all $\theta_j \approx 0$, except for θ_0 (the constant term). This makes $h_{\theta} \approx 0$ and defies the purpose of training and leads to underfitting (a flat horizontal line).

7.3 Regularized Linear Regression

7.3.1 Gradient Descent

We will modify the gradient descent function to separate out θ_0 from the rest of the parameters because we do not want to penalize θ_0 .

repeat until convergence{

$$\theta_0 := \theta_0 - \alpha \frac{1}{m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)}) x_0^{(i)}$$

$$\theta_j := \theta_j - \alpha \left[\left(\frac{1}{m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)}) x_j^{(i)} \right) + \frac{\lambda}{m} \theta_j \right]$$

$\}$, where $j \in \{1, 2, \dots, n\}$

The above equation can be re-arranged to get the final form:

$$\theta_j := \theta_j(1 - \alpha \frac{\lambda}{m}) - \frac{\alpha}{m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)})x_j^{(i)} \quad (16)$$

The term $(1 - \alpha \frac{\lambda}{m})$ will always be less than 1. Intuitively, this reduces the parameter, then the rest of equation 16 carries the normal gradient descent.

7.3.2 Normal Equation

Recall from our previous normal equation (Equation 7), we have the design matrix \mathbf{X} such that

$$\mathbf{X} = \begin{bmatrix} - & (x^{(1)})^T & - \\ - & (x^{(2)})^T & - \\ - & (x^{(3)})^T & - \\ & \vdots & \\ - & (x_m^T) & - \end{bmatrix}$$

Now, to add in regularization to Equation 7, we get:

$$\theta = ((\mathbf{X}^T \mathbf{X}) + \lambda \cdot \mathbf{L})^{-1} \mathbf{X}^T y \quad (17)$$

where $L \in \mathbb{R}^{(n+1) \times (n+1)}$

$$L = \begin{bmatrix} 0 & & & & \\ & 1 & & & \\ & & \ddots & & \\ & & & \ddots & \\ & & & & 1 \end{bmatrix} \quad (18)$$

Supopose non-invertibility arises: $m \leq n$, i.e #examples is less than or equal to number of features, then using a $\lambda > 0$ in Equation 17 will resolve the non-invertibility.

7.4 Regularized Logistic Regression

7.4.1 Regularized Logistic Cost Function

We can modify our old logistic cost function (Equation 9) to apply regularization.

$$J(\theta) = \frac{-1}{m} \sum_{i=1}^m [y^{(i)} \log h_{\theta}(x^{(i)}) + (1 - y^{(i)}) \log (1 - h_{\theta}(x^{(i)}))] + \frac{\lambda}{2m} \sum_{j=1}^n \theta_j^2 \quad (19)$$

Note that the second sum in Equation 19 explicitly exludes the bias term θ_0 .

7.4.2 Regularized Logistic Gradient Descent

The gradient descent is similar to that of linear regression; however note that the hypothesis function has been updated to Equation 8.

repeat until convergence{

$$\theta_0 := \theta_0 - \alpha \frac{1}{m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)}) x_0^{(i)}$$

$$\theta_j := \theta_j - \alpha \left[\left(\frac{1}{m} \sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)}) x_j^{(i)} \right) + \frac{\lambda}{m} \theta_j \right]$$

}